

Coulomb Correction to the Screening Angle of the Molière Multiple Scattering Theory

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Coulomb correction to the screening angular parameter of the Molière multiple scattering theory is found. Numerical calculations are presented in the range of nuclear charge $2 \leq Z \leq 82$. Comparison with the Molière result for the screening angle reveals up to 30% deviation from it for sufficiently heavy elements of the target material.

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I. INTRODUCTION

The Coulomb correction (CC) is the difference between the exact in the parameter $\xi = Z\alpha/\beta$ result and the Born approximation. At intermediate energies, when kinetic energy of the scattered particles is approximately from 0.1 to 2.0 MeV, formulas for the Coulomb corrections are not available in analytical form [1]. The analytic formulas for the high-energy CC are known as the Bethe–Bloch formulas for the ionization losses [2] and those for the Bethe–Heitler cross section of bremsstrahlung [3, 4].

A similar expression was found for the total cross section of the Coulomb interaction of compact hadronic atoms with ordinary target atoms [5]. Were also obtained CC to the cross sections of the pair production in nuclear collisions [4, 6, 7], an interaction potential [8], and the spectrum of bremsstrahlung [4, 9, 10]. The specificity of the expressions presented in this work is that they define the CC to the Born screening angle χ_a^B and an exponential part of distribution function of the Molière multiple scattering theory.

The Molière theory of multiple scattering [11] is the most used tool for taken into account the multiple scattering effects in experimental data processing. The experiment DIRAC and many others [12–16] face the problem of excluding the multiple scattering effects in matter from obtained data. As the Molière theory is currently used in the energy range roughly from 1 MeV to 200 GeV, the role of the high-energy CC to the parameters of this theory becomes significant.

Of especial importance is the Coulomb correction to the screening angular parameter, as this parameter also enters other important quantities in the Molière theory. In his original paper, Molière received an approximate semianalytical relation for the exact χ_a and first-order χ_a^B values of the screening angle:

$$\chi_a = \chi_a^B \sqrt{1 + 3.34 (Z\alpha/\beta)^2}.$$

While the first term of this expression is defined quite accurately, the coefficient in the second term is found only numerically and approximately.

In this work, we have obtained for χ_a an exact in ξ compact analytical result. In the second-order in ξ , it is given by:

$$\chi_a = \chi_a^B \sqrt{1 + 2.13 (Z\alpha/\beta)^2}.$$

We have also evaluated numerically, in the range $2 \leq Z \leq 82$, the Coulomb corrections to the Born approximations of the screening angular parameter. Additionally, we have estimated the absolute and relative accuracies of the Molière theory in determining these corrections.

The paper is organized as follows. In Section 2, we consider the standard approach to the multiple scattering theory proposed by Molière. In Section 3, we obtain the analytical and numerical results for the Coulomb corrections to the screening angular parameter. In Conclusion, we briefly summarize our results.

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II. MOLIÈRE MULTIPLE SCATTERING THEORY

Multiple scattering of a charged high-energy particle on the atoms of a target is the diffusion process in the angular plane of $(\theta, \phi) = \boldsymbol{\chi}$. The angular phase volume is $dO = 2\pi\chi d\chi$, we suppose $\chi = |\boldsymbol{\chi}| \ll 1$. We define $\sigma(\chi)\chi d\chi d\phi$ as the differential scattering cross section into the angular interval $\chi, \chi + d\chi$; the Rutherford scattering cross section reads

$$\sigma_R(\chi) = \left(\frac{2Ze^2}{mv^2} \right)^2 \frac{1}{\chi^4}, \quad U = \frac{e^2 Z}{r}, \quad e^2 = 4\pi\alpha, \quad (1)$$

where m and v are the mass of the scattered particle and its velocity at large distances from the scattering center, which assumed to be at rest; α is the fine structure constant and Z is the atomic charge number.

Define now $W(\theta, t)\theta d\theta$ as the number of electrons scattered in the angular interval $d\theta$ after traveling through the target of thickness t . The normalization condition $\int W(\theta, t)d^2\theta = 1$. The Boltzmann transport equation is

$$\frac{\partial W(\theta, t)}{\partial t} = -n_0 W(\theta, t) \int \sigma(\chi)\chi d\chi + n_0 \int W(\boldsymbol{\theta} - \boldsymbol{\chi}, t)\sigma(\chi)d^2\chi, \quad (2)$$

in which n_0 is the number of the scattered centrum in 1 cm^3 , $d^2\chi = \chi d\chi d\phi/(2\pi)$. The first term in the right-hand side describes the decreasing in the number of electrons from the cone θ , and the second the increasing in the cone from the outside of the cone.

Following the Molière, we introduce the Bessel transformation of distribution

$$g(\eta, t) = \int_0^\infty \theta J_0(\eta\theta) W(\theta, t) d\theta, \quad (3)$$

$$W(\theta, t) = \int_0^\infty \eta J_0(\eta\theta) g(\eta, t) d\eta. \quad (4)$$

For $g(\eta, t)$, using the folding theorem, we obtain

$$\frac{\partial g(\eta, t)}{\partial t} = -n_0 g(\eta, t) \int_0^\infty \sigma(\chi)\chi d\chi [1 - J_0(\eta\chi)]. \quad (5)$$

Its solution is

$$g(\eta, t) = \exp \{N(\eta) - N_0\}, \quad (6)$$

$$N(\eta) = n_0 t \int \sigma(\chi)\chi d\chi J_0(\eta\chi). \quad (7)$$

Inserting this expression in the Bessel transform of the distribution function W we have:

$$W(\theta, t) = \frac{1}{2\pi} \int_0^\infty \eta d\eta J_0(\eta\theta) \exp \left\{ -n_0 t 2\pi \int_0^\infty \sigma(\chi)\chi d\chi [1 - J_0(\eta\chi)] \right\}. \quad (8)$$

For the screening potential, the differential scattering cross section reads

$$\sigma(\chi) = \frac{4Z^2 e^4}{(vp)^2 (\chi^2 + \chi_0^2)^2}, \quad \chi_0 = \frac{\hbar}{pa}, \quad (9)$$

and the total cross becomes

$$\sigma = 2\pi \int_0^\infty \sigma(\chi)\chi d\chi = \frac{4\pi a^2 (Ze^2)^2}{(\hbar v)^2}. \quad (10)$$

In the case of a thin target $t \ll l_s$, where $l_s = 1/(n\sigma)$, the distribution function may be written as

$$W(\theta, t) = nt\sigma(\theta) = \frac{N}{S}\sigma(\theta) . \quad (11)$$

Here, N is the number of scattering centers, S is the area of the thin target surface ($N\sigma(\theta) \ll S$), and $W(\theta, t) = N\sigma(\theta)/S$ is the probability of single scattering.

For large values of χ , the cross section $\sigma(\chi) \sim 1/\chi^4$ decreases rapidly. It is a complicated function for $\chi \sim \chi_0$ with

$$\chi_0 = \frac{\lambda}{a}, \quad \lambda = \frac{\hbar}{mv}, \quad a = 0.885 a_0 Z^{-1/3} . \quad (12)$$

Here, a_0 is the Bohr radius of the particle, and a is the Fermi radius of the atom.

For the reasonable thickness, the width of the multiple scattering distribution is very large compared with χ_0 .

Let us write

$$n_0 t \sigma(\chi) \chi d\chi = 2\chi_c^2 \chi d\chi \frac{q(\chi)}{\chi^4}, \quad \chi_c^2 = 4\pi n_0 t \frac{Z(Z+1)z^2 e^4}{(pv)^2}, \quad e^2 = 4\pi\alpha, \quad (13)$$

where z is the charge of the scattered particle. $q(\chi)$ is the ratio of actual to Rutherford scattering cross sections. We replace $Z^2 \rightarrow Z(Z+1)$ keeping in mind the scattering on atomic electrons.

The physical meaning of χ_c can be understood from the requirement that the probability of scattering on the angles exceeding χ_c is unity:

$$2n_0 t \int_{\chi_c}^{\infty} d\sigma(\chi) = 2 \frac{4\pi n_0 t e^4 Z(Z+1)}{(mv^2)^2} \int_{\chi_c}^{\infty} \frac{d\chi}{\chi^3} = 1 . \quad (14)$$

Typically, $\chi_c/\chi_0 = 100$. The quantity $q(\chi)$ is equal to unity for large values of $\chi \geq \chi_c$ and tends to zero at $\chi = 0$. The main χ values belong to the region $\chi \sim \chi_0$. It contains deviation from the Rutherford formulae due to the effects of screening of atomic electrons and the Coulomb corrections arising from multiphoton exchanges between the scattered particle and the atomic nuclei.

We obtain in terms of χ_c

$$-\ln g(\eta, t) = 2\chi_c^2 \int_0^{\infty} \frac{d\chi}{\chi^3} q(\chi) [1 - J_0(\chi\eta)] . \quad (15)$$

To estimate the value of integral, we introduce (following [11, 17]) some quantity k from the region (χ_0, χ_c) :

$$\chi_0 \ll k \ll \chi_c . \quad (16)$$

In the region $\chi < k$, we can use $1 - J_0(\chi\eta) = (\chi\eta)^2/4$:

$$\int_0^k \frac{d\chi}{\chi^3} q(\chi) [1 - J_0(\chi\eta)] = \frac{1}{4}\eta^2 \int_0^k \frac{d\chi}{\chi} q(\chi) . \quad (17)$$

In the region $k < \chi$, we can put $q(\chi) = 1$:

$$\begin{aligned} \int_k^{\infty} \frac{d\chi}{\chi} [1 - J_0(\chi\eta)] &= \frac{1}{4}\eta^2 I_1(k\eta) , \\ I_1(x) &= 4 \int_x^{\infty} \frac{dt}{t^3} [1 - J_0(t)] = \frac{2}{x^2} [1 - J_0(x)] + 2 \int_x^{\infty} \frac{dt}{t^2} J_1(t) , \\ 2 \int_x^{\infty} \frac{dt}{t^2} J_1(t) &= \frac{1}{x} J_1(x) + \int_x^{\infty} \frac{dt}{t} J_0(t), \quad x = k\eta . \end{aligned} \quad (18)$$

Here, we used

$$\begin{aligned} \int_x^\infty \frac{dt}{t^2} J_1(t) &= \frac{1}{x} J_1(x) + \int_x^\infty \frac{dt}{t} J_1'(t) = \\ &= \frac{1}{x} J_1(x) + \int_x^\infty \frac{dt}{t} \left(J_0(t) - \frac{J_1(t)}{t} \right), \quad tJ_1' = tJ_0 - J_1. \end{aligned}$$

Using $\int_x^\infty J_0(t)dt/t = \ln(2/x) - C_E + O(x^2)$ at $x \ll 1$ we obtain

$$\int_x^\infty \frac{d\chi}{\chi^3} [1 - J_0(\chi\eta)] = \frac{1}{4} \eta^2 \left[1 - C_E - \ln(k\eta) + O((k\eta)^2) \right], \quad (19)$$

with the Euler constant $C_E = 0.57721 \dots$

Considering the contribution of the region $\chi < k$ Molière introduce the notion of the screening angle χ_a :

$$-\ln \chi_a = \lim_{k \rightarrow \infty} \left[\int_0^k \frac{d\chi}{\chi} q(\chi) + \frac{1}{2} - \ln k \right]. \quad (20)$$

Hence, we obtain

$$-\ln g(\eta, t) = N_0 - N(\eta) = \frac{1}{2} (\chi_c \eta)^2 \left[-\ln(\chi_a \eta) + \frac{1}{2} + \ln 2 - C_E \right]. \quad (21)$$

Introducing a new variable $y = \chi_c \eta$ we get

$$\begin{aligned} N_0 - N(\eta) &= \frac{1}{4} y^2 \left[\tilde{b} - \ln \left(\frac{1}{4} y^2 \right) \right], \\ \tilde{b} &= \ln \frac{\chi_c^2}{\chi_a^2} + 1 - 2C_E \equiv \ln \frac{\chi_c^2}{(\chi_a')^2}. \end{aligned} \quad (22)$$

The Molière transformed equation is

$$\begin{aligned} W(\theta, t) \theta d\theta &= \lambda d\lambda \int_0^\infty y dy J_0(\lambda y) \exp \left\{ \frac{1}{4} y^2 \left[-\tilde{b} + \ln \left(\frac{1}{4} y^2 \right) \right] \right\}, \\ \lambda &= \theta / \chi_c. \end{aligned} \quad (23)$$

This rather simple formula permits one us to develop an iteration procedure for W . Really, putting $\tilde{b} = B - \ln B$ and introducing the variables $x = \lambda^2/B$ and $u = y\sqrt{B}$ one can obtain the expansion of the distribution function in a power series in $1/B$:

$$W(\theta) \theta d\theta = \frac{1}{\chi_c^2 B} \theta d\theta \left[W^{(0)}(x) + \frac{1}{B} W^{(1)}(x) + \frac{1}{B^2} W^{(2)}(x) + \dots \right],$$

with

$$\begin{aligned} W^{(0)}(x) &= 2 \exp \left(-\frac{\theta^2}{\theta^2} \right), \quad W^{(1)}(x) \approx \frac{2\theta^2}{\theta^4}, \quad \dots, \\ W^{(n)}(x) &= \frac{1}{n!} \int_0^\infty u du J_0(u\sqrt{x}) \left[\frac{1}{4} u^2 \ln \left(\frac{1}{4} u^2 \right) \right]^n \exp \left\{ -\frac{1}{4} u^2 \right\}, \end{aligned}$$

$$x = \theta^2 / (\chi_c^2 B), \quad \theta^2 = x_c^2 B.$$

The result of numerical integration $W^{(n)}(x)$ was obtained in papers by Molière, Bethe and Scott [11, 17] (see also [18]). In practice, the value of B as a solution of the transcendental equation $\tilde{b} = B - \ln B$ is large enough $B \approx 5$ to provide the convergence of the expansion series.

Let us investigate the expression $\ln g = N - N_0(\eta)$:

$$\ln g = \frac{y^2}{4} \left[B - \ln B - \ln \frac{y^2}{4} \right] = \frac{y^2 B}{4} - \frac{1}{B} \left[\frac{y^2 B}{4} \ln \frac{y^2 B}{4} \right]. \quad (24)$$

Its minimal value is $\ln g_{min} = e^{\tilde{b}-1}$ corresponding to the value $y_0^2/4 = e^{\tilde{b}-1}$. Since $e^{\tilde{b}} \approx (\chi_c/\chi_a)^2$ is of the same order of magnitude as the number of collisions N_0 , the accuracy of the final result of Moliere increases with the number of collisions as $\exp\{-N_0/e\}$. As was shown by Bethe,

$$\begin{aligned} e^{\tilde{b}} &= \frac{\chi_c^2}{1.167\chi_a^2} = 4\pi N_A t \left(\frac{\hbar}{mc} \right)^2 \frac{(Z+1)Z^{1/3}z^2 0.885^2}{\beta^2 A 1.167 (1.13 + 3.76\xi^2)} = \\ &= \frac{6680 t (Z+1)Z^{1/3}z^2}{\beta^2 A (1 + 3.34\xi^2)}. \end{aligned} \quad (25)$$

Here, $\tilde{b} \approx 8.8$, $N_A = 6.02 \times 10^{23} \text{ cm}^{-3}$ is the Avogadro number, A is the atomic weight, $\xi = Z\alpha/\beta$ is the ‘Born parameter’, $\beta = v/c$, and the thickness t of the target is measured in units $\text{gramm} \times \text{cm}^2$.

Some comments. The quantity $e^{\tilde{b}} = (\chi_c/\chi_a')^2$ depends on the screening angle $\chi_a' = 1.080\chi_a$. The screening angle incorporates the deviation of the potential from the Coulomb one from both the screening effect of atomic electrons and the Coulomb corrections.

Estimating the scattering phases within the Thomas–Fermi model

$$\begin{aligned} V(r) &= \pm \frac{zZe^2}{r} \Lambda \left(\frac{r}{a} \right), \quad a = Z^{-1/3} \times 0.466 \times 10^{-8} \text{ cm}, \\ \Lambda(r') &= \sum_{i=1}^3 a_i e^{-\tilde{b}_i r'}, \\ a_1 &= 0.1, \quad a_2 = 0.55, \quad a_3 = 0.35, \\ \tilde{b}_1 &= 6, \quad \tilde{b}_2 = 1.2, \quad \tilde{b}_3 = 0.3, \end{aligned} \quad (26)$$

in the limit $a \rightarrow \infty$ or the limit of small ξ , one obtains

$$q(\chi) = \left(\frac{\chi}{\chi_0} \right)^4 \left(\sum_{i=1}^3 \frac{a_i}{\tilde{b}_i^2 + (\chi/\chi_0)^2} \right)^2. \quad (27)$$

In order to obtain a result valid for large ξ and also for large angles χ , Molière used the WKB method and rather a rough approximation in describing the Coulomb corrections. His result for the screening angle turns out to be only numerical and approximate. As a result it leads to the first term $\chi_0^2 \times 1.13$ of the expression for screening angle:

$$\chi_a^2 = \chi_0^2 (1.13 + 3.76 \xi^2). \quad (28)$$

In the next section, we will use for these purposes the eikonal approximation and obtain an exact expression describing the Coulomb correction to the value of the Born-approximation screening angle $\chi_a^B = \sqrt{1.13}\chi_0$.

III. COULOMB CORRECTION TO THE SCREENING ANGULAR PARAMETER

Remind now the relations for scattering amplitude in eikonal approximation:

$$\begin{aligned} f(\mathbf{q}) &= \frac{1}{2\pi i} \int d^2b \exp\{-i\mathbf{q}\mathbf{b}\} S(\mathbf{b}), \quad S(\mathbf{b}) = \exp\{-i\phi(\mathbf{b})\} - 1, \\ \phi(\mathbf{b}) &= \frac{1}{v} \int_{-\infty}^{\infty} dz U(\mathbf{b}, z), \quad U(\mathbf{b}, z) = Z\alpha/r, \quad r = \sqrt{b^2 + z^2}, \end{aligned} \quad (29)$$

where $\phi(\mathbf{b})$ is the eikonal phase (see [19], Appendix E).

It's convenient to define an interaction potential in the Landau–Pomeranchuk–Migdal effect theory (see Appendix A in [8]):

$$V(\mathbf{b}) = n \int \left(1 - \exp\{i \mathbf{q} \mathbf{b}\}\right) |f(\mathbf{q})|^2 d^2 q, \quad |f(\mathbf{q})|^2 d^2 q = d\sigma(\mathbf{q}).$$

In the case of the screened Coulomb potential, we have the following expression for the eikonal phase:

$$\phi(\mathbf{b}) = \frac{Z\alpha}{v} \int_{-\infty}^{\infty} dz \frac{1}{r} \exp\left\{-\frac{r}{a}\right\} = 2 \frac{Z\alpha}{v} K_0\left(\frac{b}{a}\right), \quad (30)$$

where a is the Thomas–Fermi atom radius, and $K_0(b/a)$ is the modified Bessel function.

The equation for the potential $V(\mathbf{b})$ can be written (after performing the angular integration) as

$$\frac{V(\mathbf{b})}{2\pi n} = \int [1 - J_0(qb)] d\sigma(\mathbf{q}). \quad (31)$$

Comparing this result with

$$\frac{N_0 - N(\eta)}{n_0 t} = \int [1 - J_0(\eta\chi)] d\sigma(\chi), \quad (32)$$

in which $N_0 - N(\eta) = -\ln g(\eta)$, we obtain the similarity when accept $qb = \eta\chi$, $q = p\eta$, $b = \chi/p$, $p = mv$.

So the problem of deviation of the potential $V(\mathbf{b})$ from the Born one

$$\begin{aligned} \Delta V(\mathbf{b}) &= -\Delta_{CC}[V(\mathbf{b})] = \\ &= n \int d^2 x \left[\exp\left\{i[\phi(\mathbf{b} + \mathbf{x}) - \phi(x)]\right\} - 1 + \frac{1}{2}[\phi(\mathbf{b} + \mathbf{x}) - \phi(x)]^2 \right], \end{aligned}$$

with $\Delta_{CC}[V(\mathbf{b})] \equiv V(\mathbf{b}) - V^B(\mathbf{b})$ is similar to our problem of deviation of the screening angle in the eikonal approximation from its Born value:

$$\begin{aligned} \Delta[-\ln g(\eta)] &= \Delta_{CC}[\ln g(\eta)] = \frac{1}{2}(\chi_c \eta)^2 \Delta_{CC}[\ln(\chi'_a)^2] = \\ &= (\chi_c \eta)^2 \frac{1}{2\pi} \int d^2 x \left[\left(\frac{(\mathbf{x} + \mathbf{b})^2}{x^2}\right)^{i\xi} - 1 + \frac{\xi^2}{2} \ln^2 \frac{(\mathbf{x} + \mathbf{b})^2}{x^2} \right] = \\ &= (\chi_c \eta)^2 f(\xi), \end{aligned} \quad (33)$$

with the Coulomb corrections $\Delta_{CC}[\ln g(\eta)] \equiv \ln g(\eta) - \ln g^B(\eta)$ and $\Delta_{CC}[\ln(\chi'_a)] \equiv \ln(\chi'_a) - \ln(\chi'_a)^B$.

The two-dimensional integral calculated in [8] turns out to be

$$f(\xi) = \xi^2 \sum_{n=1}^{\infty} \frac{1}{n(n^2 + \xi^2)}, \quad \xi = Z\alpha/\beta. \quad (34)$$

From (33), we obtain

$$\Delta_{CC}[\ln(\chi'_a)] = f(\xi) \quad (35)$$

or, equivalently,

$$\Delta_{CC}[\ln(\chi'_a)] = \text{Re}[\psi(1 + i\xi)] + C_E, \quad (36)$$

with $C_E = -\psi(1)$. Here, we use the smallness of the ratio $x/a \ll 1$, the $b \sim x \ll a$ and apply the relevant asymptotic of the Bessel function $K_0(z) = C - \ln(z/2) + O(z^2)$. The main reason of such derivation of relations (33) and (36) is the significantly different regions of contributions of the screening effects and Coulomb corrections. Really, the last ones play the main role in the region of small impact parameters, where the number of atom electrons is small and the screening effects are negligible. These results may also be obtained with by using the technique developed in [5].

Finally, we get

$$\chi_a^2 = 1.13\chi_0^2 \left[1 + 2.131 \left(\frac{Z\alpha}{\beta} \right)^2 + \dots \right], \quad (37)$$

which can be compared with the Molière one

$$\chi_a^2 = 1.13\chi_0^2 \left[1 + 3.34 \left(\frac{Z\alpha}{\beta} \right)^2 + \dots \right]. \quad (38)$$

To calculate the second-order relative corrections to the first-order results, $\delta_{CC}^{(2)}$ and $\delta_M^{(2)}$, which correspond to Eqs. (37) and (38), respectively, and to investigate their Z -dependence, we first present these equations in the approximate form:

$$(\chi'_a) \approx (\chi'_a)^B \left[1 + 1.204 \left(\frac{Z\alpha}{\beta} \right)^2 + O \left(\left(\frac{Z\alpha}{\beta} \right)^4 \right) \right], \quad (39)$$

$$(\chi'_a) \approx (\chi'_a)^B \left[1 + 1.670 \left(\frac{Z\alpha}{\beta} \right)^2 + O \left(\left(\frac{Z\alpha}{\beta} \right)^4 \right) \right]. \quad (40)$$

Then, (39) and (40) become

$$\delta_{CC}^{(2)}(\chi'_a) = \frac{\Delta_{CC}^{(2)}(\chi'_a)}{(\chi'_a)^B} \approx 1.204 \left(\frac{Z\alpha}{\beta} \right)^2 + O \left(\left(\frac{Z\alpha}{\beta} \right)^4 \right), \quad (41)$$

$$\delta_M^{(2)}(\chi'_a) = \frac{\Delta_M^{(2)}(\chi'_a)}{(\chi'_a)^B} \approx 1.670 \left(\frac{Z\alpha}{\beta} \right)^2 + O \left(\left(\frac{Z\alpha}{\beta} \right)^4 \right). \quad (42)$$

In order to compare our results and those of Molière, we also define the absolute $\Delta_{CCM}^{(2)}$ and relative $\delta_{CCM}^{(2)}$ differences between the values of $\delta_M^{(2)}(\chi'_a)$ and $\delta_{CC}^{(2)}(\chi'_a)$:

$$\delta_{CCM}^{(2)} = \frac{\Delta_{CCM}^{(2)}}{\delta_M^{(2)}} = \frac{\delta_{CC}^{(2)} - \delta_M^{(2)}}{\delta_M^{(2)}} = \frac{\delta_{CC}^{(2)}}{\delta_M^{(2)}} - 1. \quad (43)$$

Table 1 presents the Z -dependence of the second-order corrections to the first-order results for $\beta = 1$. It shows that the values of the relative corrections $\delta_{CC}^{(2)}$ for large- Z targets ($Z \sim 80$) does reach 40%. Hence, it is also obvious that with the rise in the nuclear charge the absolute accuracy $\Delta_{CCM}^{(2)}$ of the Molière theory in determining the relative CC to χ'_a due to the difference of the coefficients in (41) and (42) increases to approximately 16%, and the corresponding relative error $\delta_{CCM}^{(2)}$ does not depend on Z and is about 28%. During our analysis, we omit systematically the contribution of order α compared with ones of order 1.

We can also calculate the exact in ξ absolute correction $\Delta_{CC}[\ln(\chi'_a)] = f(\xi)$ and relative correction $\delta_{CC}(\chi'_a)$ to the Born screening angle $(\chi'_a)^B$,

$$\delta_{CC}(\chi'_a) = \frac{\chi'_a - (\chi'_a)^B}{(\chi'_a)^B} = \frac{\Delta_{CC}(\chi'_a)}{(\chi'_a)^B} = \exp[f(\xi)] - 1, \quad (44)$$

as well as compare δ_{CC} with the Molière result $\delta_M^{(2)}$:

$$\delta_{CCM} = \frac{\Delta_{CCM}}{\delta_M^{(2)}} = \frac{\delta_{CC} - \delta_M^{(2)}}{\delta_M^{(2)}} = \frac{\delta_{CC}}{\delta_M^{(2)}} - 1. \quad (45)$$

For this purpose, we must first calculate the values of the function $f(\xi) = \text{Re}[\psi(1 + i\xi)] + C_E$. The digamma series

$$\psi(1 + \xi) = 1 - C_E - \frac{1}{1 + \xi} + \sum_{n=2}^{\infty} (-1)^n [\zeta(n-1)] \xi^{n-1}, \quad (46)$$

where ζ is the Riemann zeta function and $|\xi| < 1$, leads to the corresponding power series for $\text{Re}[\psi(1+i\xi)] = \text{Re}[\psi(i\xi)]$ and $|\xi| < 2$:

$$\text{Re}[\psi(i\xi)] = 1 - C_E - \frac{1}{1 + \xi^2} + \sum_{n=1}^{\infty} (-1)^{n+1} [\zeta(2n+1)] \xi^{2n}, \quad (47)$$

and the function $f(\xi) = \xi^2 \sum_{n=1}^{\infty} [n(n^2 + \xi^2)]^{-1}$ can be represented at $|\xi| < 2$ as [20]

$$\begin{aligned} f(\xi) &= 1 - \frac{1}{1 + \xi^2} + \sum_{n=1}^{\infty} (-1)^{n+1} [\zeta(2n+1)] \xi^{2n} \\ &= 1 - \frac{1}{1 + \xi^2} + 0.2021 \xi^2 - 0.0369 \xi^4 + 0.0083 \xi^6 - \dots \end{aligned} \quad (48)$$

An equivalent way to estimate $f(\xi)$ to four decimal figures is to present the sum from (34) in the following form [4]:

$$\begin{aligned} \sum &= (1 + \xi^2)^{-1} + \sum_{n=1}^{\infty} (-\xi^2)^{n-1} [\zeta(2n+1) - 1], \\ &= (1 + \xi^2)^{-1} + 0.20206 - 0.0369 \xi^2 + 0.0083 \xi^4 - 0.002 \xi^6. \end{aligned} \quad (49)$$

Equation (49) is sufficient to evaluate this sum up to $\xi < 2/3 = 0.667$.

The calculation results for \sum (49), function $f(\xi)$ (48), the relative Coulomb correction δ_{CC} (44), their difference Δ_{CCM} , and relative difference δ_{CCM} (45) with the Molière correction $\delta_M^{(2)}$ (42) at $\beta = 1$ are given in Table 2.

It will be seen from Table 2 that for the light elements up to $Z = 28$, all the exact corrections coincide with the corresponding second-order corrections of Table 1. Beginning with $Z = 42$ the relative CC are lower than the above-mentioned $\delta_{CC}^{(2)}(\chi'_a) > \delta_{CC}(\chi'_a)$, and this discrepancy increases approximately to 10% for the heavy elements with $Z \sim 80$. The magnitude of $\Delta_{CC} [\ln(\chi'_a)] = f(Z\alpha)$ is about 30% for $Z \sim 80$. The size of the corresponding relative CC for these values of Z is approximately 40%. The absolute and relative differences with Molière corrections increases to 20% and 34%, respectively, at $Z \sim 80$.

Thus, in the case of scattering on large- Z targets such corrections to the Molière result (42) as Δ_{CCM} and δ_{CCM} become significant and should be taken into account in the description of experiments with nuclear targets.

IV. CONCLUSION

We have calculated the Coulomb correction $\Delta_{CC} [\ln(\chi'_a)]$ and the relative Coulomb correction $\delta_{CC}(\chi'_a)$ to the screening angle χ'_a both analytically and numerically in the range $2 \leq Z \leq 82$. We have found that these corrections are the order of 30% to 40% for $Z \sim 80$. Additionally, we evaluated the difference and relative difference between our results in determining the CC to χ'_a and those of Molière and found that they are about 20% and 30%, respectively, for heavy atoms of the target material.

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Table 1. The Z -dependence of the second-order corrections defined by Eqs. (41)–(43)

M	Z	$Z\alpha$	$\delta_{CC}^{(2)}$	$\delta_M^{(2)}$	$-\Delta_{CCM}^{(2)}$	$-\delta_{CCM}^{(2)}$
Be	4	0.029	0.001	0.001	0.000	0.286
Al	13	0.094	0.011	0.015	0.004	0.280
Ti	22	0.160	0.031	0.043	0.012	0.280
Ni	28	0.204	0.050	0.070	0.020	0.286
Mo	42	0.307	0.113	0.157	0.044	0.280
Sn	50	0.365	0.160	0.222	0.062	0.279
Ta	73	0.533	0.342	0.474	0.132	0.278
Pt	78	0.569	0.390	0.541	0.150	0.279
Au	79	0.577	0.400	0.554	0.154	0.278
Pb	82	0.598	0.431	0.598	0.166	0.279

Table 2. The Z -dependence of the exact with respect to ξ corrections (35), (44), and (45)

M	Z	$Z\alpha$	Σ	$f(Z\alpha)$	δ_{CC}	$-\Delta_{CCM}$	$-\delta_{CCM}$
Be	4	0.029	1.201	0.001	0.001	0.000	0.286
Al	13	0.094	1.193	0.011	0.011	0.004	0.280
Ti	22	0.160	1.176	0.031	0.031	0.012	0.280
Ni	28	0.204	1.160	0.049	0.050	0.020	0.287
Mo	42	0.307	1.113	0.105	0.110	0.047	0.297
Sn	50	0.365	1.080	0.144	0.154	0.068	0.306
Ta	73	0.533	0.971	0.276	0.318	0.157	0.330
Pt	78	0.569	0.947	0.307	0.359	0.182	0.336
Au	79	0.577	0.941	0.313	0.367	0.187	0.337
Pb	82	0.598	0.926	0.332	0.393	0.205	0.342